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MENDELEYEV'S PERIODIC TABLE

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/A Digest. Numbers in brackets refer to the bibliography./

/The author in this article correlates interatomic distances with chemical properties and positions in the periodic table. The controversy of the zero and eighth groups is resolved, in favor of Mendeleyev's original proposal. The author briefly mentions the application of his formulas to the transuranic elements./

To eliminate inconsistency and arbitrariness in the arrangement of elements by groups and subgroups in the periodic table, the author considers it necessary to have an accurate function which will derive specific property from atomic number and maximum valence (or the integral value of the group into which an element falls in the periodic table).

Unfortunately, no one has yet supplied such a function, but the author's reports /11-15/ are of value in calculations of atomic radii and interatomic distances of elements and their crystalline compounds. Sarkisov's equation

$$R = C_R \cdot \left(\frac{F}{f}\right)^{\frac{1}{3}} \tag{1a}$$

for atomic radii of crystals or his corresponding equation

$$d = C_d \left(\frac{F}{f}\right)^{\frac{1}{3}} \tag{1b}$$

for interatomic distances shows that one of the basic characteristics of elements -- their interatomic distances -- makes it possible to predict their chemical properties (represented in the functional relations between F and f). In equation (1), F is a function of atomic number Z; and the number f of bond electrons is determined by the group number in the periodic table, i.e., by maximum absolute valence.

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The author's equation was derived for minimum total energy of the crystal lattice. The original equation expressed the potential energy of interaction of bond electrons and nuclear electrons in the space of one elementary nucleus and the kinetic energy of interaction of such electrons:

$$E_{pot} = -\eta_1 f^2 e^2 / R$$

and

$$E_{kin} = -\eta f^{5/3} / R.$$

However, the conclusions of equation (1) are naturally vitiated by several simplifications. Thus, the author disregarded the interaction energies of electrons in their own field, i.e., energies of repulsion between bond electrons and remaining electrons and among bond electrons themselves.

Because this interaction is very complicated to calculate for total effect of repulsion, the function F in equation (1) was introduced from physical considerations by way of additional assumptions to explain experimental facts. Function F can be expressed as $Z^{2/3}$ (where Z is the total number of electrons in the atom or atomic number).

The number f of bond electrons in Subgroup-A elements was considered by the author to be the maximum number of valence electrons N or the corresponding number of the group in the periodic table; in other words, $f = N$. For all Subgroup-B elements, it was assumed that $f = 8-N$. Hydrogen and helium were considered exceptional cases where $f = 2-N$, since they are elements of the first period with the main quantum number $u = 1$, and can therefore have a maximum of two electrons.

The author's assumption for Subgroup-B elements is corroborated by the fact that the majority of these elements crystallize, so that each atom has 8-N close neighbors, whereas all Subgroup-A elements crystallize into steric-centered cubical, face-centered cubical, and hexagonal compact structures. Even in zinc and cadmium lattices, which are crystallized in a singular modification of the hexagonal compact structure similar to the simple rhombohedral structure of mercury, each atom has six close neighbors. Hume-Rothery /16/ has extended the 8-N law even to the metals Cu, Ag, Au, although their atoms are relatively difficult to arrange in the lattice so that each atom has seven strong bonds.

In equation (1) the coefficient of proportionality C for $f = 1$ and $F = 1$ numerically equals the atomic radius of hydrogen ($C_R = R_H$ and $C_d = d_H$).

Actually, the author's equation of interatomic distances of inert and other gases in their molecular lattices reveals the physical significance of the constant C_d, because in these instances one can employ the experimentally known value for the lattice constant of molecular hydrogen ($C_d = d_{H2}$). Therefore, the equation for interatomic distances in molecular-type lattices has the form:

$$d = d_{H2}\left(\frac{F}{f}\right)^{\frac{1}{3}} \tag{2}$$

Equation (2) was used to calculate the interatomic distances of the inert gases and of oxygen and nitrogen in their molecular lattices. The number of bond electrons of known metalloids was calculated for $f = 8-N$, as in the case of Subgroup-B elements. For hydrogen and helium we have $f = 2-N$. Therefore, the number f of bond electrons is 1 for hydrogen and 2 for helium, the other inert gases having $f = 8$; oxygen has $f = 2$ and nitrogen $f = 3$.

As the value of d_{H2} in equation (2), the author took the experimental value of the lattice constant of molecular hydrogen a = 3.75 A, since hydrogen crystallizes in a closely packed hexagonal lattice at $c/a = 1.63$ $d_1 = d_2 = d$. The calculated interatomic distances of the above elements for $d_{H2} = 3.75$ Å agree with the experimental values /17/ in Table 1.

All elements given in this table crystallize in a face-centered cubical lattice. Helium is not included because it crystallizes in a densely packed hexagonal lattice at $c/a = 1.63$. For helium, therefore, the experimental value of the interatomic distance is determined as d = a. The table below clearly shows the close agreement between calculated and experimental values of interatomic distances. Equation (2) may determine the hitherto-unknown value d for radon, with a somewhat smaller interatomic distance than that of xenon. Radon's smaller interatomic distance is related to the "contracting" influence of the lanthenides /14/, a phenomenon which will be discussed farther on.

Table 1. Lattices of the Molecular Type

$$(C_d = d_{H2} = 3.75 \text{ Å})$$

Elements	f	a experimental	d experimental	d calculated	Difference (%)
$H_2 - H_2$	1	3.75 Å	3.75 Å	3.75 Å	0
$N_2 - N_2$	3	5.67	4.01	4.01	0
$O_2 - O_2$	2	6.83	4.83	4.73	-2
He - He	2	3.57	3.57	3.47	-3
Ne - Ne	8	4.52	3.19	3.13	-2
Ar - Ar	8	5.40	3.82	3.56	-7
Kr - Kr	8	5.69	4.02	4.16	3
Xe - Xe	8	6.24	4.41	4.55	3
Rn - Rn	8	--	--	4.48	--

* * *

The author showed /13/ that interatomic distances in binary alloys and compounds are determined by:

$$d = C_d \frac{pF_1^{\frac{1}{3}} + (1-p)F_2^{\frac{1}{3}}}{\sqrt{pf_1 + (1-p)f_2}^{\frac{1}{3}}} \qquad (3)$$

where p represents the atomic weights. When $F_1 = F_2 = F$ and $f_1 = f_2 = f$, equation (3) is identical to (1) and gives the interatomic distances of metals:

$$d = 2R = C_d \left(\frac{F}{f}\right)^{\frac{1}{3}}$$

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Metals and alloys which crystallize into face-centered cubical lattices ($k = 12$) have the constant $C_d = 2C_R$ or $C_d = 2 \cdot 1.16 = 2.32$. Since this constant depends on structural types and bond types, in each instance a correction must be made for lattice contraction or expansion during transition to other structural types. Then

$$C_d = 2C_R \, \alpha \tag{4}$$

where α is the coefficient of contraction or expansion.

* * *

For Subgroup-A elements the integer N of a group in the periodic table corresponds to the number f of bond electrons of this subgroup in Table 2. Subgroup-B elements have $N = 8-f$ (with the exception of hydrogen and helium for which $N = 2-f$).

Because of the arrangement, two subgroups in Group 0 and Group VIII of the periodic table cannot in principle exist. In fact, if elements of Subgroup-B were in Group VIII, then we would have $N = 8-f = 8$, true only for elements with $f = 0$. Such a possibility is excluded because the author's equation gives $d = \infty$ when $f = 0$. Analogous reasoning leads to the same conclusion concerning the possible existence of Subgroup-A elements in Group 0, because then we would have $N = f = 0$ and, therefore, $d = \infty$; hence comes the failure of many authors to eliminate Group 0 by transferring the inert gases to Group VIII.

In the author's Table 2, therefore, Group 0 with $f = 0$ is properly absent; but the absence of Group 0 does not contradict the presence of a zero group in the periodic table, since the inert gases as Subgroup-B elements of Group VIII have $N = 8-f = 0$ for $f = 8$. Similarly explained is the difference in distribution of all the remaining Subgroup-B elements in these tables.

In Table 2 below, the elements with atomic numbers 90-92 are placed by the author in parentheses and the transuranic elements (93-96) are not listed; this is connected with the existence of the second "rare earth" group of elements with five f-electrons. However, Seaborg's hypothesis [23] that a new series of rare earths begins with actinium and the first five f-electrons appear at thorium is not, in the author's opinion, entirely conclusive.

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Table 2

Period	1 A	1 B	2 A	2 B	3 A	3 B	4 A	4 B	5 A	5 B	6 A	6 B	7 A	7 B	8 A	8 B
I		H 1 / 1.0		He 2 / 1.59												
II	Li 3 / 2.08	F 9 / 4.32	Be 4 / 2.52	O 8 / 4.0	B 5 / 2.92	N 7 / 3.66		C 6 / 3.30								Ne 10 / 4.64
III	Na 11 / 4.95	Cl 17 / 6.61	Mg 12 / 5.24	S 16 / 6.35	Al 13 / 5.53	P 15 / 6.08		Si 14 / 5.80								Ar 18 / 6.85
IV	K 19 / 7.12	Br 35 / 10.70	Ca 20 / 7.37	Se 34 / 10.50	Sc 21 / 7.61	As 33 / 10.30	Ti 22 / 7.85	Ge 32 / 10.05	V 23 / 8.09	Ga 31 / 9.87	Cr 24 / 8.32	Zn 30 / 9.65	Mn 25 / 8.55	Cu 29 / 9.44	Fe 26 / 8.78; Co 27 / 9.00; Ni 28 / 9.22	Kr 36 / 10.90
V	Rb 37 / 11.10	I 53 / 14.11	Sr 38 / 11.30	Te 52 / 13.91	Y 39 / 11.49	Sb 51 / 13.76	Zr 40 / 11.70	Sn 50 / 13.54	Nb 41 / 11.90	In 49 / 13.39	Mo 42 / 12.10	Cd 48 / 13.18	? 43 / 12.28	Ag 47 / 13.09	Ru 44 / 12.46; Rh 45 / 12.67; Pd 46 / 12.82	Xe 54 / 14.29

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Period																		
VI	Cs 55 14.46	Ba 56 14.64	La 57 14.81 and lanthanides	Hf 72 11.51	Ta 73 11.67	W 74 11.83	Re 75 11.98	Os 76 12.14	Ir 77 12.30	Pt 78 12.46	Au 79 12.61	Hg 80 12.77	Tl 81 12.92	Pb 82 13.07	Bi 83 13.23	Po 84 13.37	? 85 13.52	Rn 86 13.67
VII	? 87 13.82	Ra 88 13.99	Ac 89 14.12	(Th) 90 14.28	(Pa) 91 14.42	(U) 92 14.58												

Lanthanides:

Ce 58 13.98	Pr 59 13.56	Nd 60 13.25	? 61 12.98	Sm 62 12.75	Eu 63 12.53	Gd 64 12.34	Tb 65 12.17	Dy 66 12.00	Ho 67 11.85	Er 68 11.71	Tu 69 11.58	Yb 70 11.46	Cp 71 11.34

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Conclusions

1. Most modified versions of the periodic table -- in particular those based on the atom's electron structure -- change Mendeleyev's natural arrangement of the elements.

2. Although many elements possess multiple valency, positive valence (which corresponds to Mendeleyev's group numbers) is an important criterion in the determination of an element's properties.

3. The author derived a universal equation without arbitrary constants to prove mathematically the arrangement of elements into groups and subgroups as proposed by Mendeleyev.

4. Mendeleyev's arrangement made the author's contribution possible.

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